

1-Perfluorobutanesulfonic acid

375-73-5 | DTXSID5030030

Model Performance

Model

Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.87	0.81	0.87	0.82	0.86	0.86

Model Results

Predicted value: 1.42 mol/L

Global applicability domain: Outside

Local applicability domain index: 2.41e-01

Confidence level: 6.23e-01

Nearest Neighbors from the Training Set

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Methylarsonic acid

Measured: 1.83

Predicted: N/A

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Monosodium
methanearsonate

Measured: 3.58

Predicted: N/A

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4-Methylbenzenesulfonic
acid

Measured: 3.60

Predicted: 2.37

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Methanesulfonic acid

Measured: 10.4

Predicted: 6.76